Renormalization Group Methods for Electronic Structure

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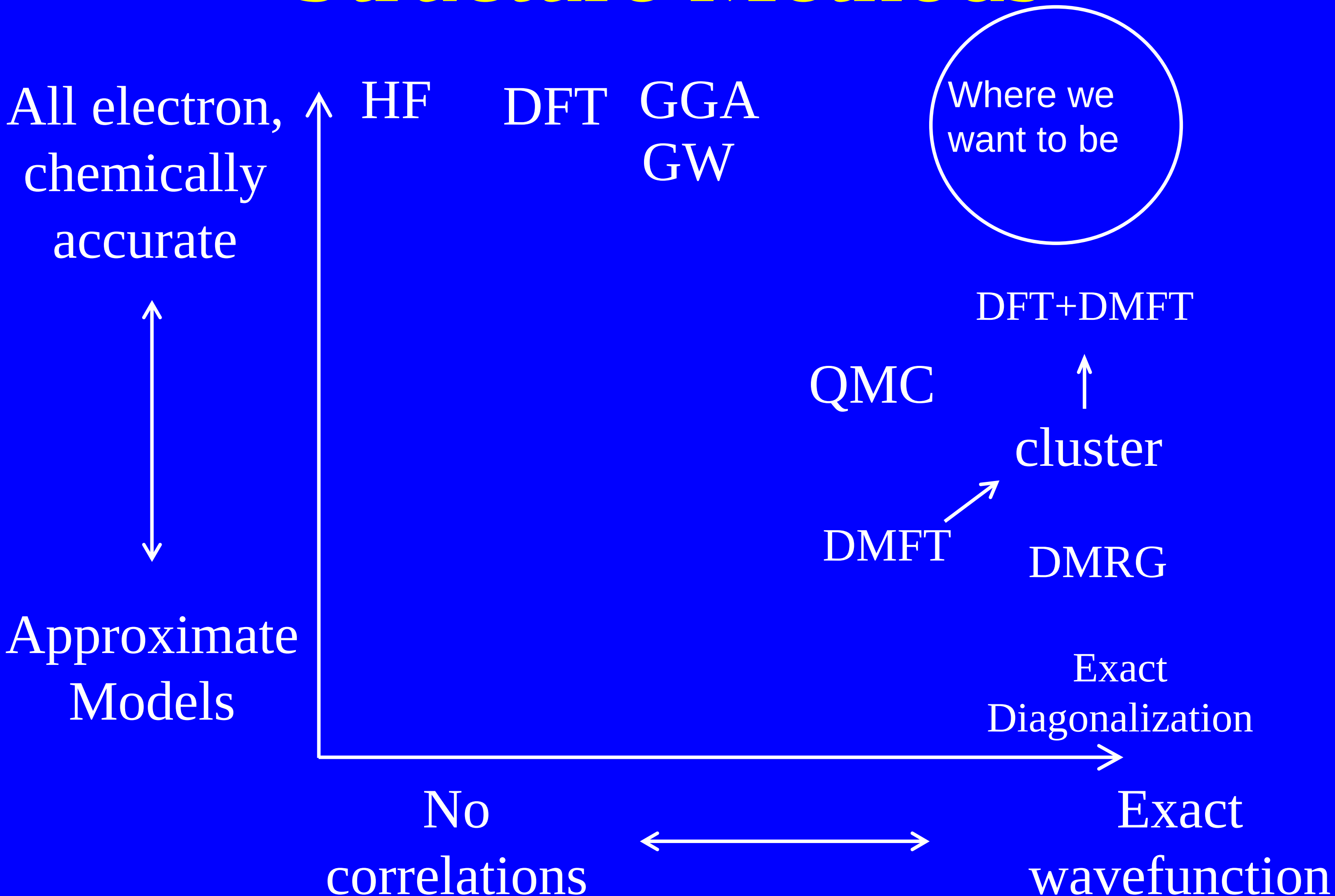
What I used to look like

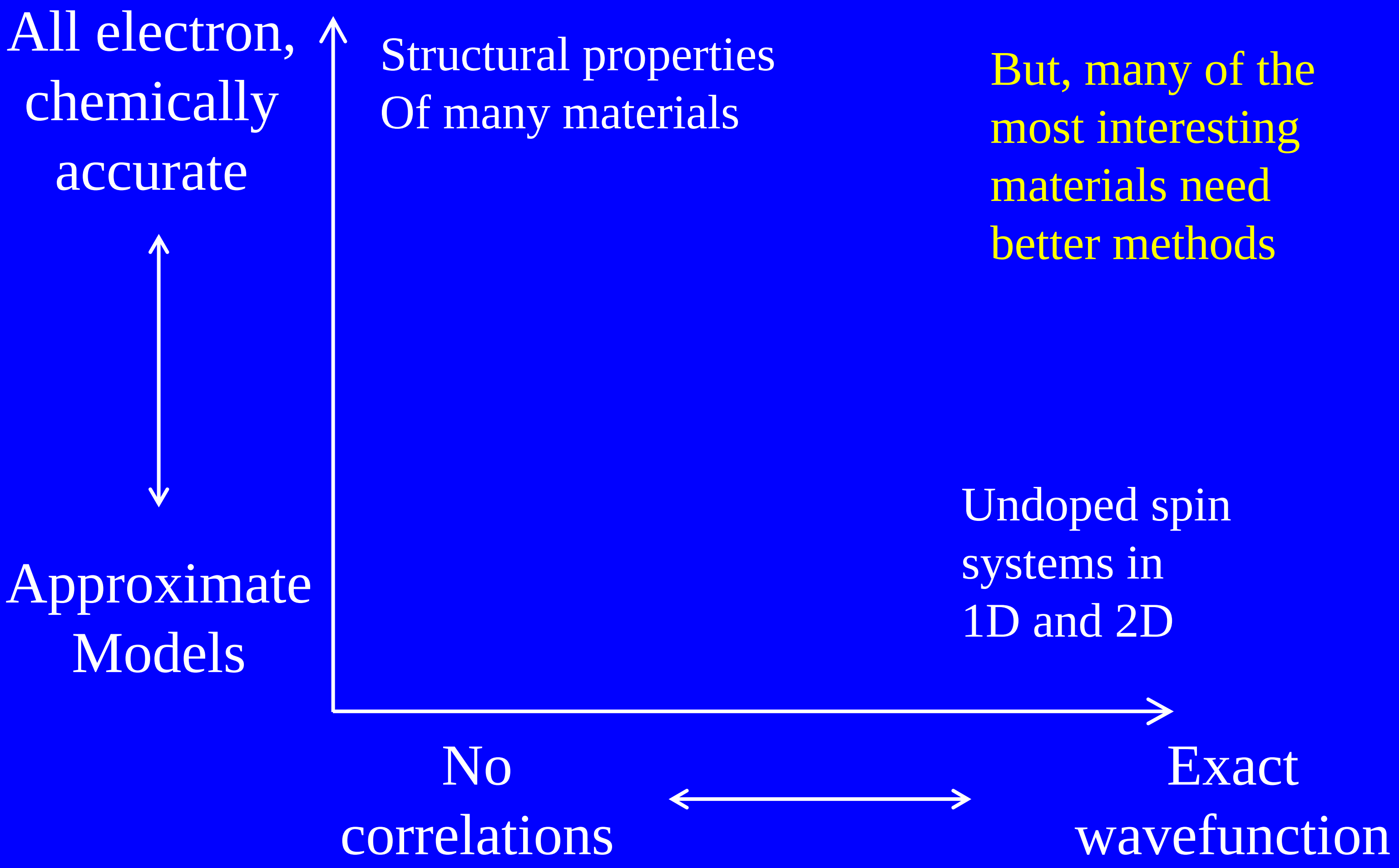
Outline

- Overview of electronic structure methods
- DMRG for quantum chemistry
- Canonical Diagonalization for downfolding

Overview of Electronic Structure Methods



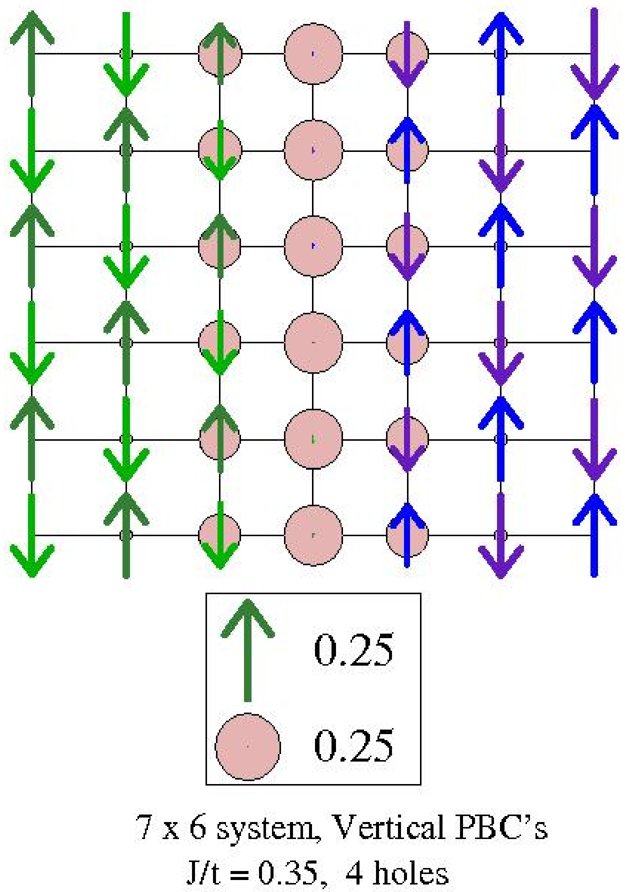
Current methods are fine for some materials

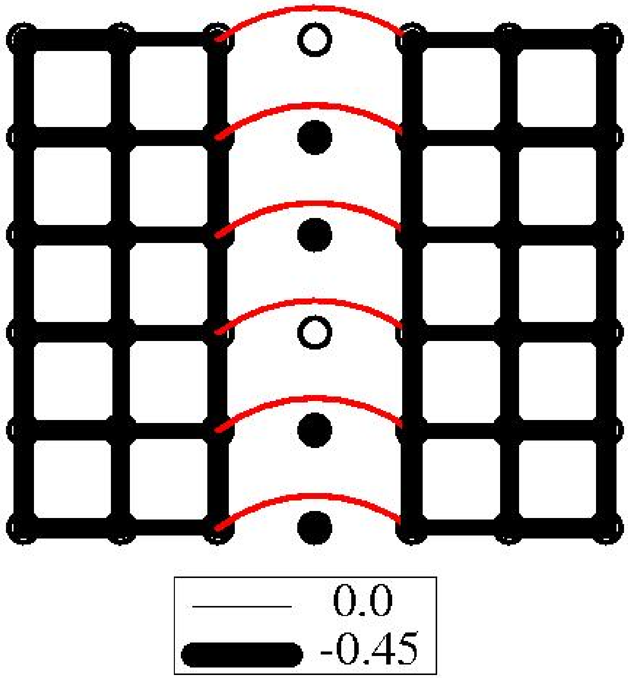


Weaknesses of Strong Correlation Methods

- Exact diagonalization: very small clusters
- DMRG: dimensionality: 1D great, 3D impossible, 2D difficult
- DMFT: lack of detailed spatial correlations (wants 3D+)
- Cluster DMFT: Is the spatial resolution good enough? Sign problem?
- QMC: Needs a good variational wavefunction

Stripes in the t-J model: an example of complicated spatial correlations

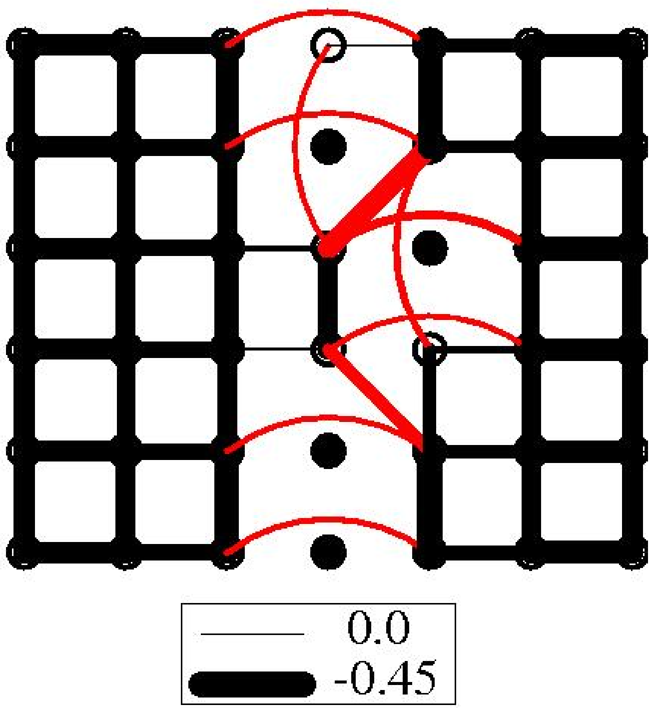




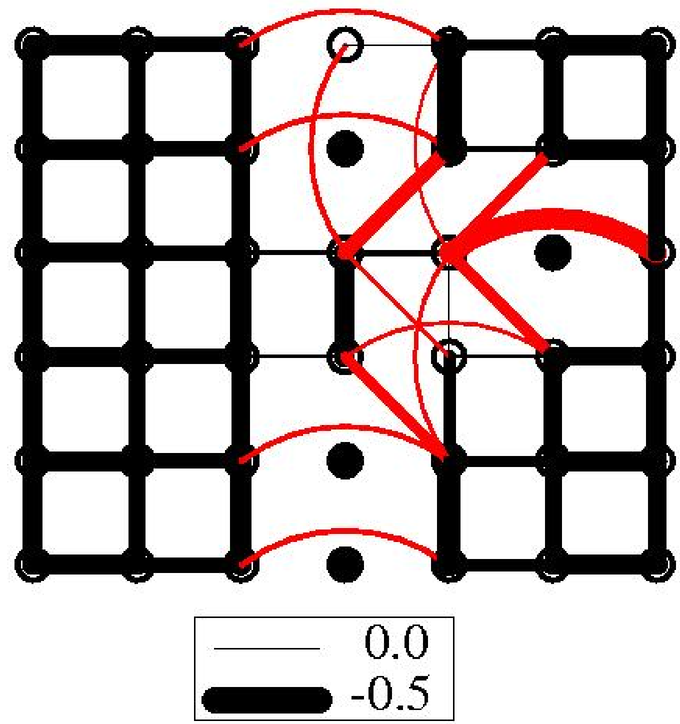
The width of the lines gives |<S(i) S(j) P(h)>| where P(h) projects the holes to the black circle sites.

<P(h)> = 0.0004

Hole motion induces a complicated distortion of the spin background



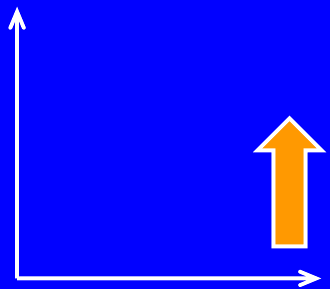
One hole hops to the right
<P(h)> = 0.00035



Two hops. <P(h)>=0.0001

Red indicates a nnn AF bond. The correlations are a combination of string motion and RVB singlets.

DMRG for quantum chemistry

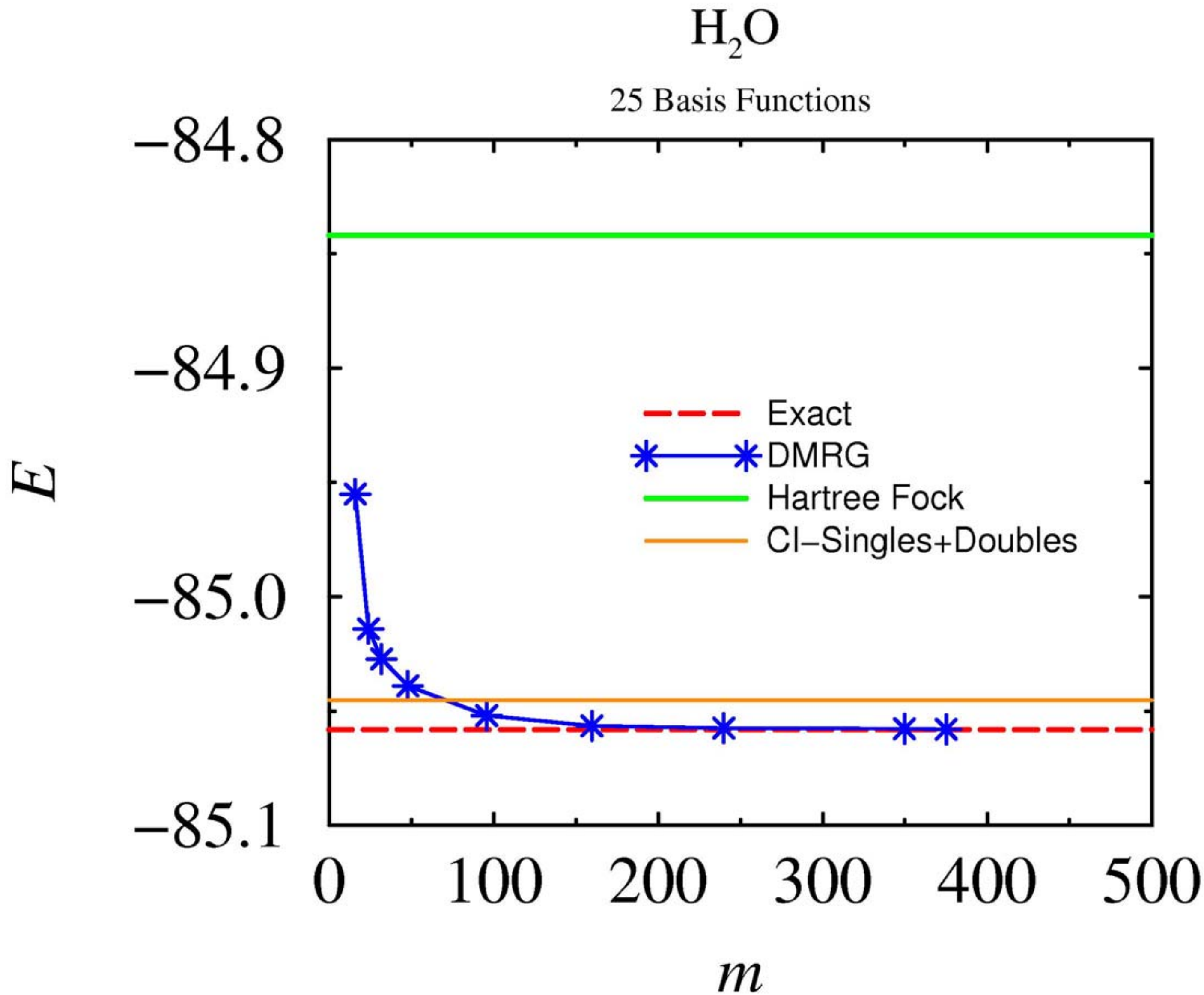


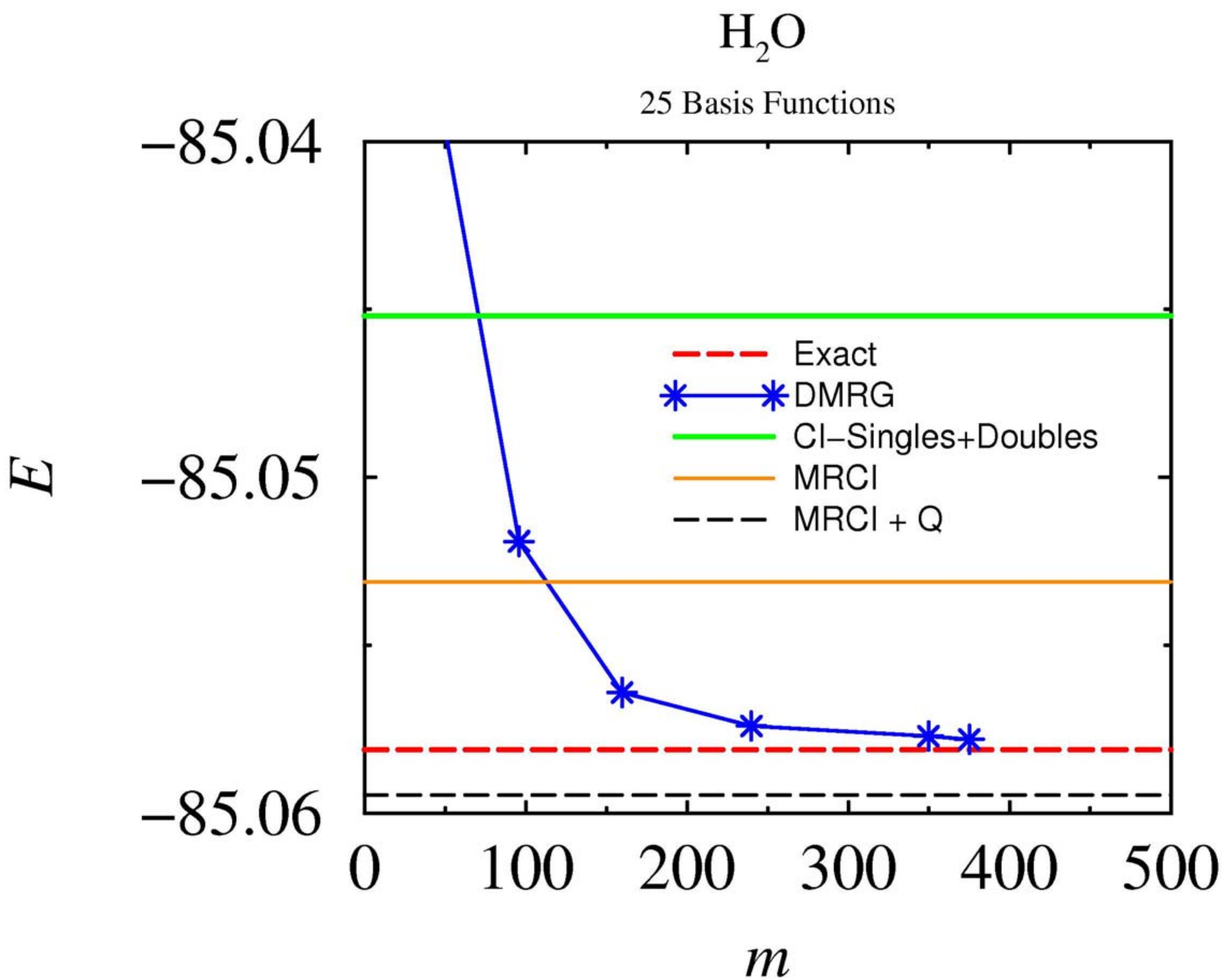
- We can regard a many-electron molecule in a basis as a lattice model with complicated interactions.
- DMRG can (in principle) be applied to any lattice model—only question is practicality.
- The difficulty for DMRG is the N^4 terms in H. There are tricks to speed things up…

QC DMRG—technical details

- Within standard QC basis, perform HF/SCF. Transform all integrals to HF basis, obtaining second quantized Hamiltonian operator. (Same for all QC correlation methods.)
- Choose an order for the sites, either by energy or to minimize strength of long range interactions.
- Apply DMRG to these artificial sites (orbitals). Accuracy depends on ordering, localization of basis, etc.
- Final calculation time: $N^3 m^3 + N^4 m^2$, where m is the number of states kept, N number of sites.

QC DMRG on a water molecule





H2O
25 Basis Functions
−85.04
−85.05
−85.06
E
0
100
200
300
400
500
m
Exact
DMRG
CI−Singles+Doubles
MRCI
MRCI + Q

Canonical Diagonalization

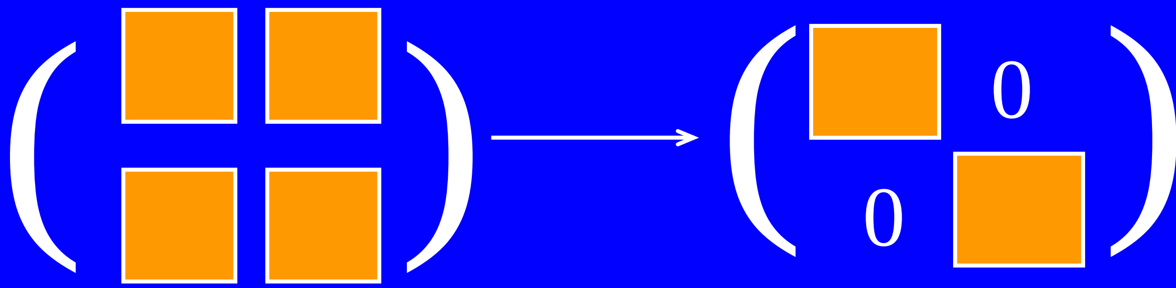
- We envision a two step process to electronic structure:
- 1. Controlled RG procedure to “downfold” accurately from a realistic all-electron system to a “model” with a few degrees of freedom—we want to remove orbitals far from the Fermi surface.
- 2. The “model” is treated with a strong correlation method (e.g. DMRG, DMFT).

Canonical Diagonalization (cont)

- How to eliminate degrees of freedom? RG tells us to integrate out degrees of freedom from H (or action S).
- CD does this via canonical (orthogonal) transformations (Schrieffer-Wolff, etc. as discussed by Jim Gubernatis!) but does it numerically (Wegner, Glazek and Wilson) on the coefficients of the second quantized Hamiltonian.
- We need to throw away many electron terms—the key approximation.

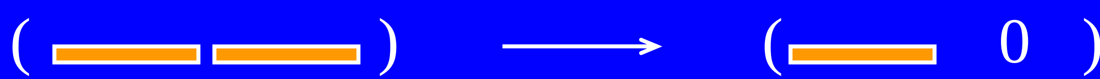
CD (cont)

Example: block diagonalizing a matrix.



$H' = O\,H\,O^T = \exp(A)\,H\,\exp(-A)$; A antisymmetric

This procedure also zeros out blocks of the eigenstates



In CD, we transform to drive the occupancy of the uninteresting orbitals to zero (or two for core orbitals).

CD (cont)

For example, to remove

$$V = ac^\dagger_{i\uparrow} c^\dagger_{j\downarrow} c_{k\downarrow} c_{l\uparrow},$$

and its Hermitian conjugate from the Hamiltonian, we construct the antihermitian operator

$$A = \theta(V - V^\dagger)/a$$

and rotate using

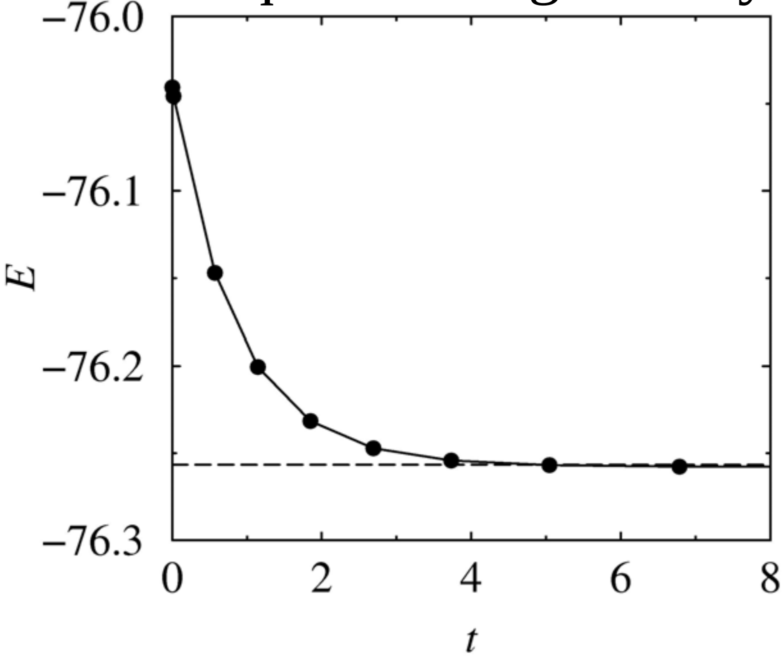
$$e^A H e^{-A} = H + [A, H] + \frac{1}{2!}[A, [A, H]] + ...$$

We can approximate θ as

$$\theta = \frac{1}{2}\tan^{-1}[2a/(E_i - E_j)].$$

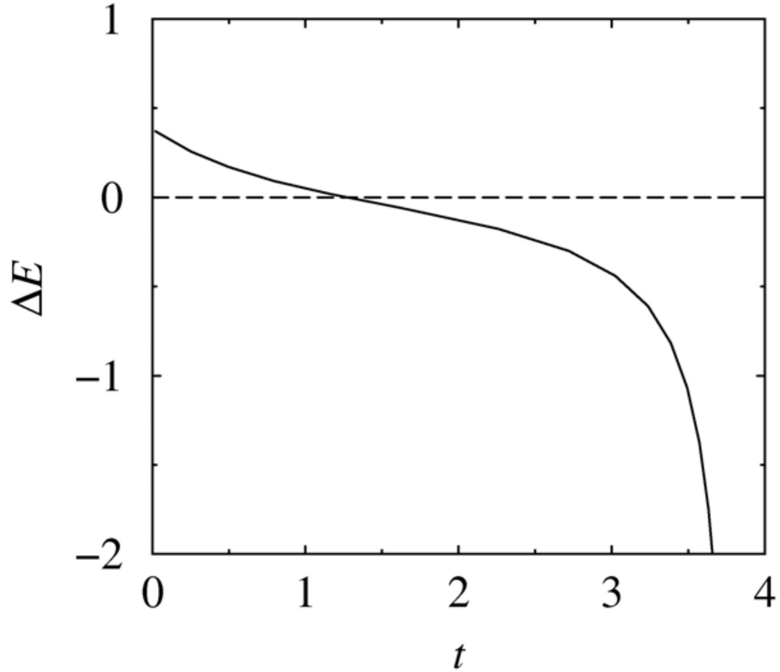
CD applied to a water molecule

H_2O, as before
Equilibrium geometry



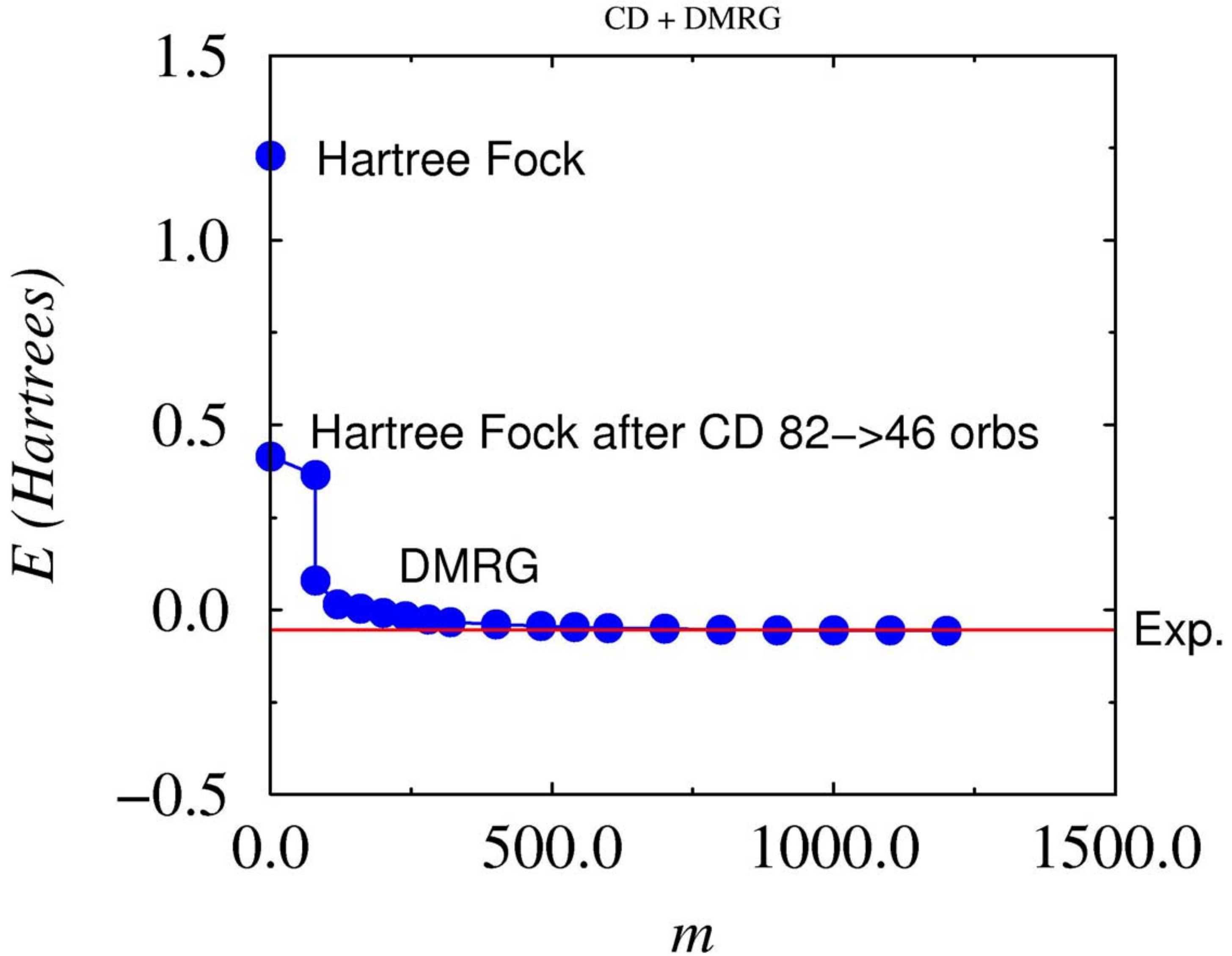
In a non-strongly-correlated System it gives excellent results.

Bonds stretched by a factor of two



It cannot handle strong correlation on its own.

CD + DMRG applied to Cr dimer



CD applied to solids

- Uncharted territory!
- Do we need a Wannier basis, or can it be done in the band states?
- How many basis states can we handle?
- Can CD be coupled with a version of DFT to remove some of the highest energy orbitals first?
- CD can be followed by DMRG, QMC, DCA, etc. But, the model will have complicated two-particle terms—can we deal with them?

Conclusions

- CD is a potentially controlled and rigorous procedure to “downfold”.
- Each many-particle method has its strength areas and weaknesses. DMRG is especially useful for low dimensional systems.
- DMRG is very useful for small molecules, but CD + DMRG is potentially much more powerful.